Transport characteristics of L-point and Γ-point electrons through GaAs–$Ga_{1-x}Al_xAs$–GaAs(111) double heterojunctions[a)]

C. Mailhiot, D. L. Smith, and T. C. McGill

T. J. Watson, Sr., Laboratory of Applied Physics, California Institute of Technology, Pasadena, California 91125

(Received 25 January 1983; accepted 21 March 1983)

We present here a study on the transport characteristics of L-point and Γ-point derived electrons through abrupt GaAs–$Ga_{1-x}Al_xAs$–GaAs(111) double heterojunctions. The use of complex-**k** band structures in the tight-binding approximation and transfer matrices provide a reasonably accurate description of the wave function at the GaAs–$Ga_{1-x}Al_xAs$ interface. A representation of the wave function in terms of bulk complex-**k** Bloch states is used in the GaAs regions where the potential is bulklike. A representation of the wave function in terms of planar orbitals is used in the central $Ga_{1-x}Al_xAs$ region where the potential deviates from its bulk value (i.e., interfacial region). Within this theoretical framework, realistic band structure effects are taken into account and no artificial rules regarding the connection of the wave function across the interface are introduced. The ten-band tight-binding model includes admixture in the total wave function of states derived from different extrema of the GaAs conduction band. States derived from the same extremum of the conduction band appear to couple strongly to each other, whereas states derived from different extrema are found to couple weakly. Transport characteristics of incoming L-point and Γ-point Bloch states are examined as a function of the energy of the incoming state, thickness of the $Ga_{1-x}Al_xAs$ barrier, and alloy composition x. Transmission through the $Ga_{1-x}Al_xAs$ barrier is either tunneling or propagating depending on the nature of the Bloch states available for strong coupling in the alloy. Since Bloch states derived from different extrema of the conduction band appear to couple weakly to each other, it seems possible to reflect the low velocity L-point component of the current while transmitting the high velocity Γ-point component.

PACS numbers: 73.40.Lq

I. INTRODUCTION

The introduction of new device fabrication technologies has allowed the realization of planar electronic devices in which the dimension perpendicular to the growth plane is of the order of a few lattice spacings. The understanding of the transport of electrons through semiconductor interfaces is of great importance regarding the performance of these very small-scale electronic devices. The major reason that makes GaAs a prime candidate for high speed electronic devices is the very high velocities that can be achieved by electrons derived from the Γ-point conduction band minimum. The small value of the Γ-point effective mass is in major part responsible for the very high velocities that can be achieved by these electrons. At higher energies, electrons start to populate the low velocity L-point and X-point GaAs conduction band valleys, therefore reducing the population of the high velocity Γ-point minimum. This has the direct effect of setting an upper limit to the speed at which the device can operate. The study of transport of electrons associated with the various GaAs conduction band valleys is therefore of crucial importance. The work presented here is concerned with the transport of L-point and Γ-point derived electron states through a GaAs–$Ga_{1-x}Al_xAs$–GaAs(111) double heterojunction structure (DHS). The transport in these structures is either tunneling or propagating depending on the nature of the states with strong coupling available for transmission in the $Ga_{1-x}Al_xAs$ barrier (i.e., evanescent or propagating). In the former, the Bloch states with strong coupling available for transmission in the $Ga_{1-x}Al_xAs$ barrier are evanescent and the wave vector **k** is complex. In the latter, the Bloch states with strong coupling available for transmission in the alloy are propagating and the wave vector **k** takes on real values.

In the following, we examine DHS in which the perpendicular dimension of the central barrier region is of the order of a few atomic layers. Since the potential varies over distances on an atomic scale, a theoretical approach beyond the effective-mass theory is needed. The theoretical framework used here exploits the bulk properties of the constituent semiconductors forming the DHS. The transport of electrons through a region of space in which the energy of the state is such that free propagation is not allowed is best described in terms of the complex-**k** bulk band structure. The breakdown of translational invariance induced by the interface implies a new set of boundary conditions that do not exclude the component of the wave vector **k** normal to the interface to take on complex values. The problem of calculating the transport coefficients of Bloch states at an abrupt interface using complex-**k** band structure, cast in a tight-binding band calculation scheme, has been addressed in the past.[1-4] The major result of the following theoretical study is that the mixing between L-point and Γ-point states appears to be small. Therefore, there seems to exist two distinctive energy barriers for L-point and Γ-point electrons. Given an alloy composition of the $Ga_{1-x}Al_xAs$ barrier, there is a range of energies for which the electrons incoming from the Γ-point minimum of GaAs are mostly transmitted, whereas the electrons incoming from the L-point extremum of GaAs are mostly reflected. It seems then possible to reflect back the low velocity L-point component of the current while allowing the high velocity Γ-point component to be transmitted.

The paper is organized as follows: in Sec. II, the basic ingredients of the theoretical technique used to calculate the transport coefficients are presented. The major results are presented and discussed in Sec. III. A summary and conclusions are given in Sec. IV.

II. CALCULATIONAL METHOD

The DHS studied consists of a region of $Ga_{1-x}Al_xAs$ located between two semi-infinite layers of GaAs. Figure 1 shows the energy band diagram and the physical configuration of the DHS. The energy band diagram of the structure indicates the relative positions of the Γ-point and the L-point conduction band edges for an alloy composition of $x \approx 0.3$ in the $Ga_{1-x}Al_xAs$ barrier. An electron incoming in the bulk region I (GaAs) at a total energy E above the GaAs Γ-point minimum is scattered at the boundaries of the barrier region II ($Ga_{1-x}Al_xAs$) and is finally transmitted in another bulk region III (GaAs). The incoming electron is derived from the Γ point or from the L point in GaAs. The Γ-point conduction band offset ΔE_Γ is a fraction of the difference in the Γ-point conduction band gaps between GaAs and $Ga_{1-x}Al_xAs$. Depending on whether we describe the total wave function in a bulk region or an interfacial region, different representations are used accordingly. We now discuss these two representations.

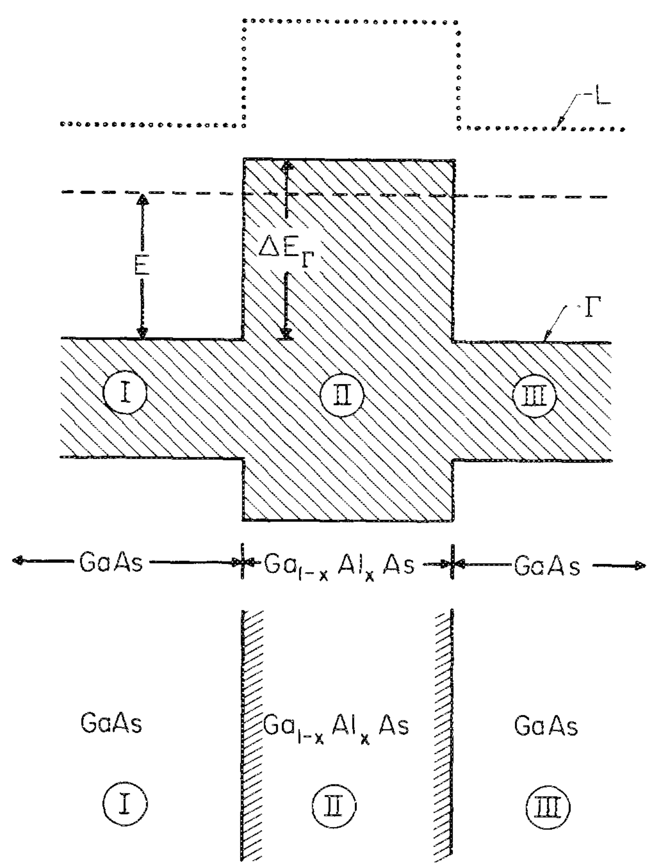

FIG. 1. Energy band diagram of GaAs–$Ga_{1-x}Al_xAs$–GaAs DHS and corresponding physical structure. The electron is derived from the Γ-point or from the L-point and has a total energy E measured with respect to the GaAs Γ-point conduction band minimum. The relative positions of the Γ-point (solid line) and the L-point (dotted line) conduction band edges are also shown for an alloy composition of $x \approx 0.3$ in the $Ga_{1-x}Al_xAs$ barrier. The Γ-point conduction band offset is indicated by ΔE_Γ.

Systems which exhibit two-dimensional periodicity are best described in a planar orbital representation.[5–10] A planar orbital is a two-dimensional Bloch sum consisting of localized atomic functions. Let $\hat{\mathbf{z}}$ be the direction normal to the interface and $\mathbf{k}_\parallel = \hat{\mathbf{x}}k_x + \hat{\mathbf{y}}k_y$ be the two-dimensional wave vector parallel to the interface. We assume that space lattice matching at the interface is such that $\mathbf{k}_\parallel$ is a good quantum number for the planar orbital. Let $\phi_{\alpha j}(\mathbf{k}_\parallel;\sigma)$ designate the planar orbital corresponding to a given atomic orbital of symmetry α within the atomic plane j of the layer σ. The bulk Bloch states $\psi(\mathbf{k}_\parallel,k_z)$, labeled by the wave vector $\mathbf{k} = \mathbf{k}_\parallel + \hat{\mathbf{z}}k_z$, are expanded in terms of this set of planar orbitals $\{\phi_{\alpha j}(\mathbf{k}_\parallel;\sigma)\}$. For interface systems, k_z is complex in general.

Wherever the total Hamiltonian is bulklike, the wave function is expanded in a set of bulk Bloch states $\{\psi(\mathbf{k}_\parallel,k_z)\}$. At the GaAs–$Ga_{1-x}Al_xAs$ interfaces, the potential is no longer bulklike and a description in terms of bulk Bloch states is prohibited. In the interfacial regions, the wave function is described in a planar orbital representation $\{\phi_{\alpha j}(\mathbf{k}_\parallel;\sigma)\}$. The connection between the bulk Bloch states representation $\{\psi(\mathbf{k}_\parallel,k_z)\}$ and the planar orbital representation $\{\phi_{\alpha j}(\mathbf{k}_\parallel;\sigma)\}$ is described in Ref. 6 and will not be repeated here.

The total number N of Bloch states $\psi(\mathbf{k}_\parallel,k_z)$ with $k_z = k_\lambda (\lambda = 1,...,N)$ corresponding to a given parallel wave vector $\mathbf{k}_\parallel$ and total energy E depends on the particular tight-binding model used and on the orientation of the interface plane. More specifically, the total number of Bloch states $\psi(\mathbf{k}_\parallel,k_\lambda)$ with real or complex wave vector k_λ is equal to the product of the number of atomic orbitals per atom times the number of layers interacting with a given layer.[1] In the tight-binding representation used here, we have five orbitals per atom ($\alpha = s^*,s,p_x,p_y,p_z$)[11] and only first nearest-neighbor interactions were included. There are therefore ten Bloch states ($N = 10$) for each parallel wave vector $\mathbf{k}_\parallel$ and total total energy E. Half of the states have to be discarded because they either grow away from the interface, if $\mathrm{Im}(k_z)$ does not have the proper sign, or are propagating in the wrong direction when k_z is real.

Let the incoming Bloch state $\psi(\mathbf{k}_\parallel,k_0)$ with real wave vector k_0 be incident from the left in GaAs onto the GaAs–$Ga_{1-x}Al_xAs$ interface. The total wave function on a given layer σ can be written as[1]:

$$\Psi(\mathbf{k}_\parallel,E;\sigma) = \psi(\mathbf{k}_\parallel,k_0;\sigma) + \sum_{k_\lambda} A_{k_\lambda}^{(\mathrm{I})}(\mathbf{k}_\parallel,E)\psi(\mathbf{k}_\parallel,k_\lambda;\sigma), \quad \text{region I} \tag{1a}$$

$$\Psi(\mathbf{k}_\parallel,E;\sigma) = \sum_{\alpha j} B_{\alpha j}^{(\mathrm{I-II})}(\mathbf{k}_\parallel,E,\sigma)\phi_{\alpha j}(\mathbf{k}_\parallel;\sigma), \quad \text{interface I–II} \tag{1b}$$

$$\Psi(\mathbf{k}_\parallel, E;\sigma) = \sum_{k_\lambda} A^{(\mathrm{II})}_{k_\lambda}(\mathbf{k}_\parallel, E)\psi(\mathbf{k}_\parallel, k_\lambda;\sigma), \text{ region II} \tag{1c}$$

$$\Psi(\mathbf{k}_\parallel, E;\sigma) = \sum_{\alpha j} B^{(\mathrm{II-III})}_{\alpha j}(\mathbf{k}_\parallel, E,\sigma)\phi_{\alpha j}(\mathbf{k}_\parallel;\sigma), \text{ interface II–III} \tag{1d}$$

$$\Psi(\mathbf{k}_\parallel, E;\sigma) = \sum_{k_\lambda} A^{(\mathrm{III})}_{k_\lambda}(\mathbf{k}_\parallel, E)\psi(\mathbf{k}_\parallel, k_\lambda;\sigma). \text{ region III.} \tag{1e}$$

The expansion coefficients $A^{(\mathrm{I})}_{k_\lambda}(\mathbf{k}_\parallel, E)$, $A^{(\mathrm{II})}_{k_\lambda}(\mathbf{k}_\parallel, E)$, and $A^{(\mathrm{III})}_{k_\lambda}(\mathbf{k}_\parallel, E)$ are associated with the bulk Bloch states representation $\{\psi(\mathbf{k}_\parallel, k_z)\}$ in regions I–III, respectively. The expansion coefficients $B^{(\mathrm{I-II})}_{\alpha j}(\mathbf{k}_\parallel, E,\sigma)$ and $B^{(\mathrm{II-III})}_{\alpha j}(\mathbf{k}_\parallel, E,\sigma)$ are associated with the planar orbital representation $\{\phi_{\alpha j}(\mathbf{k}_\parallel;\sigma)\}$, across the interfaces. At fixed total energy E and parallel wave vector $\mathbf{k}_\parallel$, we denote by $R_\lambda(\mathbf{k}_\parallel, E)$ and $T_\lambda(\mathbf{k}_\parallel, E)$ the k_z-resolved reflection and transmission coefficients corresponding to the Bloch state $\psi(\mathbf{k}_\parallel, k_\lambda)$ in GaAs. The k_z-resolved transport coefficients $R_\lambda(\mathbf{k}_\parallel, E)$ and $T_\lambda(\mathbf{k}_\parallel, E)$ are related to the expansion coefficients in the bulk Bloch state representation $A^{(\mathrm{I})}_{k_\lambda}(\mathbf{k}_\parallel, E)$ and $A^{(\mathrm{III})}_{k_\lambda}(\mathbf{k}_\parallel, E)$, respectively. The total transport coefficients $R(\mathbf{k}_\parallel, E)$ and $T(\mathbf{k}_\parallel, E)$ are just the sum of the transport coefficients $R_\lambda(\mathbf{k}_\parallel, E)$ and $T_\lambda(\mathbf{k}_\parallel, E)$. Flux conservation requires $R(\mathbf{k}_\parallel, E) + T(\mathbf{k}_\parallel, E) = 1$.

As shown in Ref. 1, the transmission coefficient for the Bloch state $\psi(\mathbf{k}_\parallel, k_\lambda)$ vanishes when the wave vector of the incoming Bloch state, k_0, approaches a critical point such that $[\partial E(\mathbf{k})/\partial k_z]_{k_z = k_0} = 0$. In that case, the incoming state is identical with the reflected state. At this critical point, the incoming state $\psi(\mathbf{k}_\parallel, k_0)$ has no component of the group velocity perpendicular to the interface and does not couple to any Bloch states in $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$. Therefore, transmission starts to occur as the incident wave vector k_0 moves away from the critical point.

The transport states in the complex-$\mathbf{k}$ band structure of GaAs and GaAs–$\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$. The complex-$\mathbf{k}$ band structure for GaAs and AlAs is well known.[1,12] We have used similar techniques to obtain the complex-$\mathbf{k}$ band structure for $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ within the virtual crystal approximation. Within the ten-band tight-binding description used here, the GaAs Γ-point conduction band minimum is $E_\Gamma^{\mathrm{GaAs}} = 1.509$ eV above the GaAs Γ-point valence band maximum and the GaAs L-point conduction band valley is at an energy $E_L^{\mathrm{GaAs}} = 0.50$ eV above the GaAs Γ-point conduction band minimum.

The propagating or evanescent nature of the Bloch states depends on the real or complex character of the wave vector k_z normal to the (111) interface plane. Propagating Bloch states are associated with real values of k_z, whereas evanescent Bloch states are associated with complex values of k_z. We denote the bulk states with $k_z = k_\lambda$ in spatial region μ by $\psi(\mathbf{k}_\parallel, k_\lambda^\mu)$. In the discussion that follows, the incident Bloch state is derived either from near the GaAs conduction band L point with real wave vector $k_0 \equiv k_L^{\mathrm{I}}$, e.g., $\psi(\mathbf{k}_\parallel, k_0) \equiv \psi(\mathbf{k}_\parallel, k_L^{\mathrm{I}})$, or from the GaAs conduction band Γ point with real wave vector $k_0 \equiv k_\Gamma^{\mathrm{I}}$, e.g., $\psi(\mathbf{k}_\parallel, k_0) \equiv \psi(\mathbf{k}_\parallel, k_\Gamma^{\mathrm{I}})$.

Throughout the calculations, the conduction band offset ΔE_Γ is taken to be equal to 85% of the difference of the Γ-point band gap between GaAs and GaAs–$\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$.[13,14] The virtual crystal approximation is used to weight the tight-binding parameters of $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ according to the alloy composition x. In the following, we consider alloy compositions in the range $x \leqslant 0.3$, for which $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ is direct. Within this composition range, the dependence of the Γ-point and L-point energy edges in $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ on the alloy composition x is, in the virtual crystal approximation: $E_\Gamma^{\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}} \approx 1.35\,x$ eV and $E_L^{\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}} \approx (0.50 + 0.65x)$eV, above the GaAs Γ-point conduction band minimum.

Throughout this study, we neglect carrier scattering by the electron–phonon interaction and by the alloy disorder. Such scattering would undoubtedly occur in the structures we consider here and will have some influence on the transport in them. We point out, however, that the thickness of the barrier in the structures we discuss is less than the scattering mean free path.[15] The scattering processes could be discussed in perturbation theory using the wave functions we calculate here as the unperturbed states.

III. RESULTS

We present the main results for the transmission coefficients of electrons derived from the L point and Γ point of GaAs through the GaAs–$\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$–GaAs(111)DHS. We discuss the transport across the central $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier as a function of the total energy E of the incoming state, thickness of the $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier, and alloy composition x.

The different transport regimes (tunneling and propagating) can be demonstrated by studying the transmission coefficient for fixed barrier thickness as a function of the energy of the incoming state. Figure 2 shows the transmission coefficient $T(\mathbf{k}_\parallel, E)$ as a function of the energy E of the incoming Bloch state. The incoming Bloch state is either derived from the GaAs L point $(k_0 \equiv k_L^I)$, or from the GaAs Γ point $(k_0 \equiv k_\Gamma^I)$. Energy is measured with respect to the GaAs Γ-point conduction band minimum. We consider the case of vanishing parallel wave vector $\mathbf{k}_\parallel = 0$. Calculations were carried out for an alloy composition of $x = 0.1$ and a barrier thickness of seven $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ layers. For the $x = 0.1$ alloy, the $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ Γ-point and the L-point energies are: $E_\Gamma^{\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}} = 0.135$ eV, and $E_L^{\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}} = 0.565$ eV, above the GaAs Γ-point conduction band minimum. For energies of the incoming states near a given GaAs conduction band extremum (L or Γ), transmission through the $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier appears to occur mostly via the coupling to states that connect to the alloy conduction band at the same extremum in the Brillouin zone (L or Γ). Since the Bloch states derived from different extrema of the conduction band appear to couple weakly to each other, the energy barrier for the states derived from the L point is different than the energy barrier for the states derived from the Γ point.

The figure clearly demonstrates that there seems to exist a range of energies above the GaAs L-point valley (E_L^{GaAs}) and

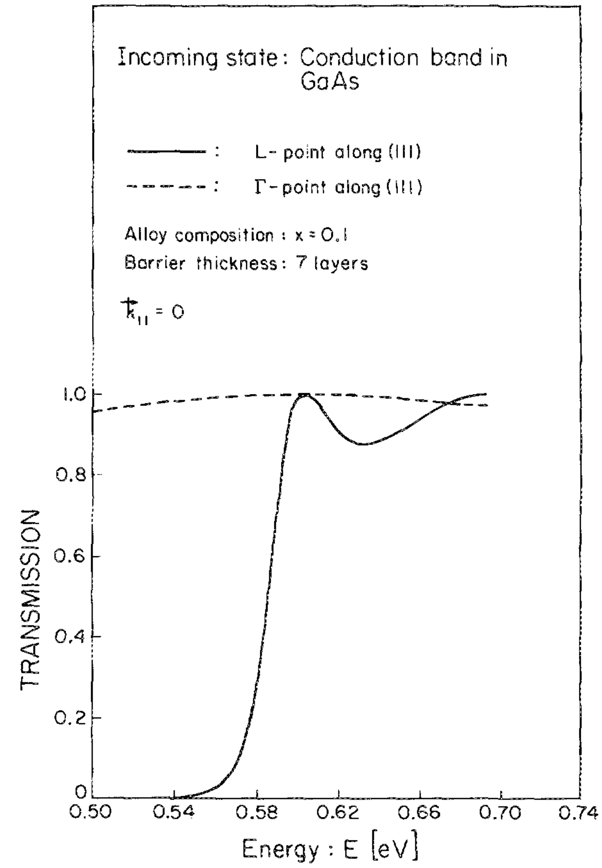

FIG. 2. Transmission coefficient $T(\mathbf{k}_{\parallel},E)$ as a function of the energy E of the incoming electron. The incoming electron is either derived from the GaAs L point (solid line), or from the GaAs Γ point (dashed line). The alloy composition of $x = 0.1$ and the $Ga_{1-x}Al_xAs$ barrier is seven layers thick. Energy is measured with respect to the GaAs Γ-point conduction band minimum and $\mathbf{k}_{\parallel} = 0$.

below the $Ga_{1-x}Al_xAs$ L-point valley ($E_L^{Ga_{1-x}Al_xAs}$), such that transmission is large for incoming Bloch states derived from the Γ point and small for incoming Bloch states derived from the L point. In this energy range, $E_L^{GaAs} < E < E_L^{Ga_{1-x}Al_xAs}$, Bloch states incoming from the Γ point in GaAs couple mostly to *propagating* Γ-point states in the barrier (k_Γ^{II} real), and Bloch states incoming from the L-point in GaAs couple mostly to *evanescent* L-point states in the barrier (k_L^{II} complex). The energy range for which the transmission $\psi(\mathbf{k}_{\parallel},k_\Gamma^I)\rightarrow\psi(\mathbf{k}_{\parallel},k_\Gamma^{III})$ is much greater than the transmission $\psi(\mathbf{k}_{\parallel},k_L^I)\rightarrow\psi(\mathbf{k}_{\parallel},k_L^{III})$ roughly corresponds to the composition-dependent L-point energy barrier that the incoming L-point Bloch states have to overcome in order for them to become propagating (k_L^{II} real) in the barrier. For the $x = 0.1$ alloy, the L-point valley of the alloy lies at $E_L^{Ga_{1-x}Al_xAs} = 0.565$ eV above the GaAs conduction band minimum, and $\psi(\mathbf{k}_{\parallel},k_L^I)\rightarrow\psi(\mathbf{k}_{\parallel},k_L^{III})$ transmission will remain small below this energy, whereas $\psi(\mathbf{k}_{\parallel},k_\Gamma^I)\rightarrow\psi(\mathbf{k}_{\parallel},k_\Gamma^{III})$ transmission will be important. Thus, for a given $Ga_{1-x}Al_xAs$ composition x, there is a range of energies, roughly $E_L^{GaAs} < E < E_L^{Ga_{1-x}Al_xAs}$, for which electrons incoming in GaAs from the Γ point are mostly transmitted whereas electrons incoming in GaAs from the L point are mostly reflected. Generally, when an incoming state in GaAs is derived from a conduction band extremum, say λ, such that $k_0 \equiv k_\lambda^I$ and E is close to E_λ^{GaAs}, the mode of transport (i.e., tunneling or propagating) appears to be determined by the nature of the states in $Ga_{1-x}Al_xAs$ derived from the same conduction band extremum $\psi(\mathbf{k}_{\parallel},k_\lambda^{II})$. For incoming state energies less than the alloy conduction band edge $E_\lambda^{Ga_{1-x}Al_xAs}$, the states that couple strongly in the alloy are gap states [$\psi(\mathbf{k}_{\parallel},k_\lambda^{II})$ evanescent] and hence the wave function is damped in the barrier. However, for incoming state energies greater than the alloy conduction band edge $E_\lambda^{Ga_{1-x}Al_xAs}$, the states that couple strongly in the alloy are band states [$\psi(\mathbf{k}_{\parallel},k_\lambda^{II})$ propagating] and hence the wave function is not damped in the barrier.

We now discuss the energy dependence of the transmission for incoming electrons derived from the GaAs L-point valley. As mentioned in Sec. II, the transmission coefficient vanishes for incoming states derived from the L point at an energy equal to the L-point extremum of GaAs, E_L^{GaAs}. At this energy, the component of the group velocity normal to the interface vanishes $[\partial E(\mathbf{k})/\partial k_z]_{k_z = k_L^I} \equiv 0$, and the incoming state $\psi(\mathbf{k}_{\parallel},k_L^I)$ does not couple to any Bloch states in $Ga_{1-x}Al_xAs$. The overall energy dependence is found to be similar to that of plane waves incident on a rectangular barrier as derived from a one-dimensional quantum-mechanical treatment.[16] For incoming states derived from the GaAs L point with energy below $E_L^{Ga_{1-x}Al_xAs} = 0.565$ eV, transport through the barrier is tunneling and the transmission is small. However, for incoming states derived from the GaAs L point with energy above $E_L^{Ga_{1-x}Al_xAs}$, transport through the barrier is propagating and the transmission becomes important. For a fixed barrier thickness, propagating transport exhibits maximum transmission whenever the energy of the incoming state is such the thickness of the $Ga_{1-x}Al_xAs$ barrier contains an integral number of half-wavelengths in the barrier region. At energies $E > E_L^{Ga_{1-x}Al_xAs}$, the transmission oscillates as a function of energy and is maximum at resonance. The off-resonance transmission amplitude increases with increasing incoming energy.

The different transport regimes (tunneling and propagating) can also be demonstrated by studying the transmission coefficient for fixed incoming energy as a function of the barrier thickness. Figure 3 shows the transmission coefficient $T(\mathbf{k}_{\parallel},E)$, as a function of the number of layers forming the central $Ga_{1-x}Al_xAs$ barrier for various energies of the incoming Bloch state. The alloy composition is $x = 0.1$ and $\mathbf{k}_{\parallel} = 0$. Layers are measured in units of $a/\sqrt{3}$, where a is the GaAs lattice constant. For the $x = 0.1$ alloy, the Γ-point and L-point conduction band energies in $Ga_{1-x}Al_xAs$ are: $E_\Gamma^{Ga_{1-x}Al_xAs} = 0.135$ eV and $E_L^{Ga_{1-x}Al_xAs} = 0.565$ eV, above the GaAs Γ-point conduction band minimum. The incoming Bloch state is either derived from the GaAs point L ($k_0 \equiv k_L^I$), or from the GaAs Γ point ($k_0 \equiv k_\Gamma^I$). For the case where the incoming Bloch state is derived from the GaAs L-point valley, the different types of transport (tunneling and propagating) are shown for an energy $E = 0.54$ eV $< E_L^{Ga_{1-x}Al_xAs}$, in which case the transport is tunneling

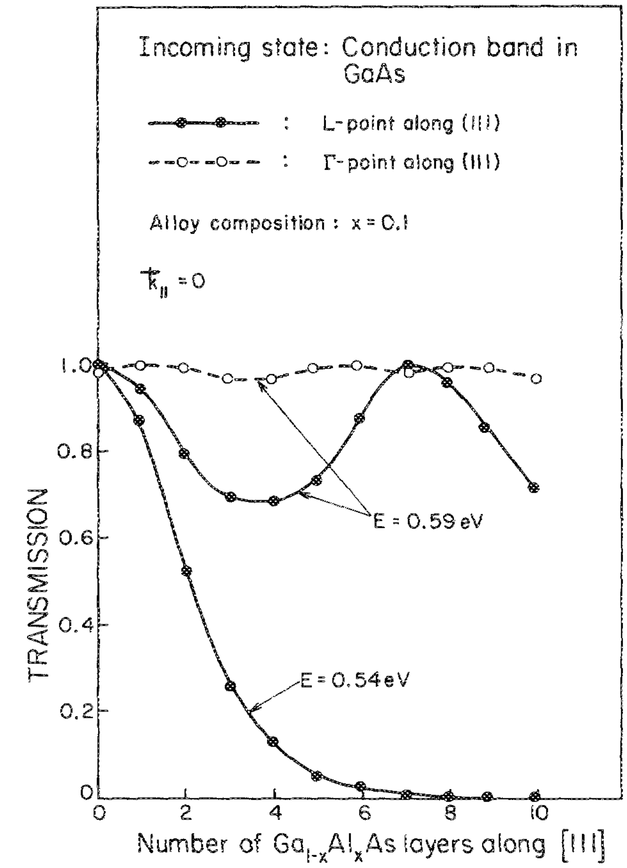

FIG. 3. Transmission coefficient $T(\mathbf{k}_{\parallel},E)$ as a function of the number of layers forming the central $Ga_{1-x}Al_xAs$ barrier for various energies of the incoming electron. The incoming electron is either derived from the GaAs L point (solid line), or from the GaAs Γ point (dashed line). The alloy composition is $x = 0.1$. Energy is measured with respect to the GaAs Γ-point conduction band minimum and $\mathbf{k}_{\parallel} = 0$. Layers are measured in units of $a/\sqrt{3}$, where a is the GaAs lattice constant.

and for an energy $E = 0.59$ eV $> E_L^{Ga_{1-x}Al_xAs}$, in which case the transport is propagating.

We discuss first the case of incoming electrons derived from the GaAs L-point valley. In the tunneling regime of transport ($E < E_L^{Ga_{1-x}Al_xAs}$), transmission occurs mostly via the coupling to *evanescent* states (k_L^{II} complex) derived from the L point of $Ga_{1-x}Al_xAs$. As seen in Fig. 3, the evanescent character of the wave function in $Ga_{1-x}Al_xAs$ is reflected in the fact that the transmission coefficient $T(\mathbf{k}_{\parallel},E)$ is an exponentially decaying function of the $Ga_{1-x}Al_xAs$ barrier thickness. These results are similar to those obtained from the thick-barrier WKB approximation.[17,18] In the propagating regime of transport ($E > E_L^{Ga_{1-x}Al_xAs}$), transmission occurs mostly via the coupling to *propagating* states (k_L^{II} real) near the conduction band L point of $Ga_{1-x}Al_xAs$. For energies of the L-point incoming electron greater than $E_L^{Ga_{1-x}Al_xAs}$, the transmission coefficient is a periodic function of the $Ga_{1-x}Al_xAs$ barrier thickness. The period is determined by the wave vector $q_L^{II} \equiv k_L^0 - k_L^{II}$, where k_L^0 is the L-point Brillouin zone edge. The transmission coefficient is unity when the thickness of the $Ga_{1-x}Al_xAs$ barrier contains an integral number of half-wavelengths (determined by q_L^{II}) in the barrier region. Since the wave vector q_L^{II} increases with the energy of the incoming L-point Bloch state, the period of the transmission amplitude decreases with the energy of the incident L-point electron. The off-resonance transmission amplitudes increase with increasing incident energy. The general qualitative behavior of the transport is similar to that exhibited by plane wave states incident on a rectangular quantum-mechanical barrier. Similar regimes of transport have also been reported for incoming states near the GaAs Γ point for GaAs–$GaAs_{1-x}P_x$–GaAs strained (100)DHS[4] and for GaAs–$Ga_{1-x}Al_xAs$–GaAs(100)DHS.[19]

Also shown in Fig. 3 is a comparison between the transmission for incoming electrons derived from the GaAs Γ point and from the GaAs L point at the same energy, namely $E = 0.59$ eV. At this energy, k_Γ^{II} and k_L^{II} are real and, consequently, the Bloch states $\psi(\mathbf{k}_{\parallel},k_\Gamma^{II})$ and $\psi(\mathbf{k}_{\parallel},k_L^{II})$ are propagating. At a given layer thickness, the transmission is greater for states incoming from the GaAs Γ point than for the states derived from the L point. This is due to the fact that, for a given energy of $E = 0.59$ eV, the Γ-point states lie at an energy of about 0.46 eV above the Γ-point minimum of the alloy, $E_\Gamma^{Ga_{1-x}Al_xAs} = 0.135$ eV. On the other hand, the L-point states lies at an energy of only 0.03 eV above the L-point valley of the alloy $E_L^{Ga_{1-x}Al_xAs} = 0.565$ eV. As seen in the figure, it seems possible to tune the thickness of the $Ga_{1-x}Al_xAs$ barrier in such a way as to reduce the transmission for the incoming states derived from the GaAs L point while the transmission for the Γ point remains close to unity.

Figure 4 shows the transmission coefficient $T(\mathbf{k}_{\parallel},E)$ as a function of alloy composition for two different $Ga_{1-x}Al_xAs$ barrier thicknesses. The incoming Bloch state is either derived from the GaAs L point ($k_0 \equiv k_L^I$), or from the GaAs Γ point ($k_0 \equiv k_\Gamma^I$). The incoming Bloch state has $\mathbf{k}_{\parallel} = 0$. The energy of the incoming state is $E = 0.501$ eV above the GaAs Γ-point conduction band minimum. As mentioned above, the Γ-point and L-point energy edges, $E_\Gamma^{Ga_{1-x}Al_xAs}$ and $E_L^{Ga_{1-x}Al_xAs}$, scale linearly with the alloy composition for $x \leqslant 0.3$. The composition x is therefore directly related to the Γ-point and L-point barrier heights at the interface. For the range of alloy compositions studied, the Γ-point and the L-point energies of $Ga_{1-x}Al_xAs$ vary in the range $0\ \text{eV} \leqslant E_\Gamma^{Ga_{1-x}Al_xAs} \leqslant 0.405$ eV and $0.50\ \text{eV} \leqslant E_L^{Ga_{1-x}Al_xAs} \leqslant 0.70$ eV, above the GaAs Γ-point conduction band minimum. For a fixed energy of $E = 0.501$ eV, the transport is propagating for Bloch states incoming from the Γ point although it is mostly tunneling for Bloch states incoming from the L point in the composition range $x \leqslant 0.3$. This is due to the fact that, in this composition range, we have $E_\Gamma^{Ga_{1-x}Al_xAs} < E < E_L^{Ga_{1-x}Al_xAs}$ so that k_Γ^{II} is real whereas k_L^{II} is mostly complex.

We first discuss the case of incoming electrons derived from the GaAs L-point valley. As the Al concentration increases, the L-point energy edge in $Ga_{1-x}Al_xAs$, $E_L^{Ga_{1-x}Al_xAs}$, increases and so does the magnitude of $\mathrm{Im}(k_L^{II})$. Therefore, the L-point derived states have smaller decay lengths and tunnel less efficiently across the

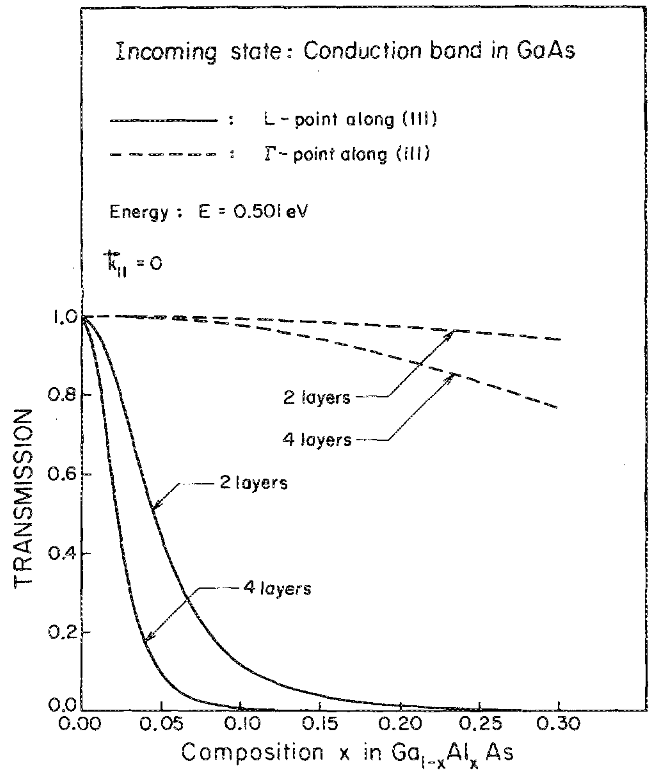

FIG. 4. Transmission coefficient $T(\mathbf{k}_{\parallel},E)$ as a function of alloy composition for two different $Ga_{1-x}Al_xAs$ barrier thicknesses. The incoming electron is either derived from the GaAs L point (solid line), or from the GaAs Γ point (dashed line). The energy of the incoming state is $E = 0.501$ eV above the GaAs Γ-point conduction band minimum and $\mathbf{k}_{\parallel} = 0$. Layers are measured in units of $a/\sqrt{3}$, where a is the GaAs lattice constant.

barrier. This, in turn, implies an increased reflection probability for the L-point derived states. At a given alloy composition x, the transmission is greater for the states incoming from the GaAs Γ point than for the states derived from the L point. This is due to the fact that the Γ-point states are transmitted in the propagating regime $(E > E_{\Gamma}^{Ga_{1-x}Al_xAs})$, whereas the L-point states are transmitted in the tunneling regime $(E < E_{L}^{Ga_{1-x}Al_xAs})$.

Since the mixing between L-point and Γ-point states appears to be small, there seems to exist two distinctive energy barriers for L-point and Γ-point electrons. In light of the results presented above, it seems possible to create a situation (by either selecting the energy, the barrier thickness, or the alloy composition) such that both the Γ-point and the L-point states were propagating in GaAs but only the Γ-point states would be propagating in $Ga_{1-x}Al_xAs$, the L-point states being evanescent in the barrier. Such a situation may have applications in GaAs high speed low power devices to provide a way of reflecting back the low velocity L-point component of the current while allowing the high velocity Γ-point component to be transmitted.

IV. SUMMARY AND CONCLUSION

We have calculated the transport coefficients of L-point Γ-point electrons through GaAs–$Ga_{1-x}Al_xAs$–GaAs(111) double heterojunctions within a ten-band tight-binding formalism. The model takes into account band effects through the use of complex-**k** band structures and transfer matrix methods reasonably well. Within this theoretical framework, k_z-resolved transport coefficients can be calculated. This, in turn, allows for a better understanding of the transmission coefficients of electrons derived from different extrema of the conduction band in GaAs. Calculation of transport coefficients associated with various conduction band valleys were carried out as a function of (1) energy of the incoming electron, (2) thickness of the central $Ga_{1-x}Al_xAs$ barrier, and (3) alloy composition x in the central $Ga_{1-x}Al_xAs$ barrier.

States originating from the same extremum of the conduction band appear to couple strongly to each other, whereas states derived from different extrema are found to couple weakly. For energies of the incoming states near a given GaAs conduction band extremum (L or Γ), transmission through the $Ga_{1-x}Al_xAs$ barrier occurs mostly via the coupling to states (evanescent or propagating) that connect to the alloy conduction band at the same extremum (L or Γ). Transmission through the $Ga_{1-x}Al_xAs$ barrier is either tunneling or propagating depending on the nature of the Bloch states available for strong coupling in the alloy. Since the mixing between L-point and Γ-point states appears to be small, there seems to exist two distinctive energy barriers for L-point and Γ-point electrons. This observation may lead to interesting effects in GaAs high speed low power electronic devices whereby the low velocity L-point component of the current could be blocked (i.e., small transmission below the L-point barrier) while the high velocity Γ-point component could be transmitted (i.e., large transmission above the Γ-point barrier).

ACKNOWLEDGMENTS

One of us (CM) has been supported by the NSERC of Canada and by the Fonds FCAC pour l'aide et le soutien à la recherche of Québec.

[a] Work supported in part by the Army Research Office under Contract No. DAAG29-80-C-0103.

[1] G. C. Osbourn and D. L. Smith, Phys. Rev. B **19**, 2124 (1979).
[2] G. C. Osbourn and D. L. Smith, J. Vac. Sci. Technol. **16**, 1529 (1979).
[3] G. C. Osbourn, J. Vac. Sci. Technol. **17**, 1104 (1980).
[4] G. C. Osbourn, J. Vac. Sci. Technol. **19**, 592 (1981).
[5] Y. C. Chang and J. N. Schulman, Phys. Rev. B **25**, 3975 (1982).
[6] J. N. Schulman and Y. C. Chang, Phys. Rev. B (to be published).
[7] D. H. Lee and J. D. Joannopoulos, Phys. Rev. B **23** 4988, 4997 (1981).
[8] J. Pollmann and S. Pantelides, Phys. Rev. B **18**, 5524 (1978).
[9] D. H. Lee and J. D. Joannopoulos, J. Vac. Sci. Technol. **19**, 355 (1981).
[10] Y. C. Chang and J. N. Schulman, J. Vac. Sci. Technol. **21**, 540 (1982).
[11] P. Vogl, H. P. Hjalmarson, and J. D. Dow, J. Phys. Chem. Sol. (in press).
[12] J. N. Schulman and Y. C. Chang, Phys. Rev. B **24**, 4445 (1981).
[13] H. C. Casey and M. B. Panish, *Heterostructure Lasers* (Academic, New York, 1978), Part A, Chap. 4.
[14] R. Dingle, W. Weigmann, and C. Henry, Phys. Rev. Lett. **33**, 827 (1974).
[15] S. M. Sze, *Physics of Semiconductor Devices*, 2nd ed. (Wiley–Interscience, New York, 1981), p. 850.
[16] L. I. Schiff, *Quantum Mechanics*, 3rd ed. (McGraw–Hill, New York, 1968), pp. 102–104.
[17] W. A. Harrison, Phys. Rev. **123**, 85 (1961).
[18] C. B. Duke, *Tunneling Phenomena in Solids* (Plenum, New York, 1969), p. 31.
[19] C. Mailhiot, T. C. McGill, and J. N. Schulman, J. Vac. Sci. Technol. B **1**, 439 (1983).